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**Electronic structure and charge injection across transition metal dichalcogenide heterojunctions: theory and experiment.**[1] ZHIXIAN ZHOU, HSUN-JEN CHUANG, Wayne State University, JIE GUAN, DAVID TOMANEK, Michigan State University — We combine *ab initio* density functional electronic structure calculations for an $NbSe_2/WSe_2$ bilayer with quantum transport measurements of the corresponding heterojunction between a few-layer $WSe_2$ semiconductor and a metallic $NbSe_2$ layer. Our theoretical results suggest that, besides a rigid band shift associated with charge transfer, the presence of $NbSe_2$ does not modify the electronic structure of $WSe_2$. Since the two transition metal dichalcogenides are structurally similar and display only a small lattice mismatch, their heterojunction can efficiently transfer charge across the interface. These findings are supported by transport measurements for $WSe_2$ field-effect transistors with $NbSe_2$ contacts, which exhibit nearly ohmic behavior and phonon-limited mobility in the hole channel, indicating that the contacts to $WSe_2$ are highly transparent.

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